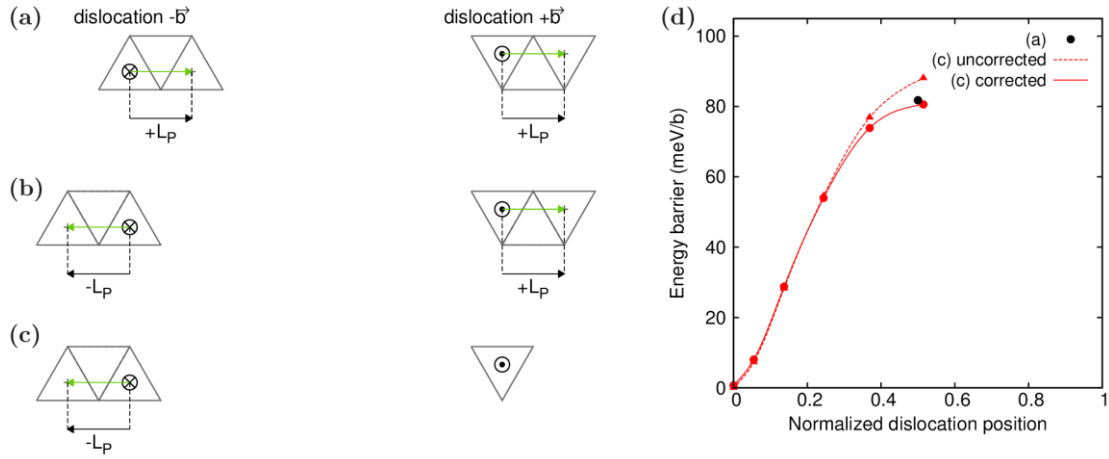**Supplementary Figure 1: Dislocation trajectories under applied stress.** Comparison of the trajectories obtained with two methods: the cost function method and the stress-based method in absence (a) and in presence (b) of applied stress. In absence of stress, the trajectories were symmetrized to show the full paths, while under stress, such symmetrization is not possible and only the calculated half paths are shown.
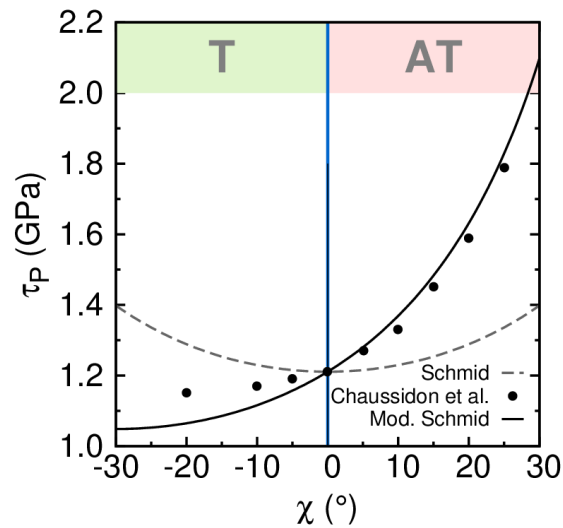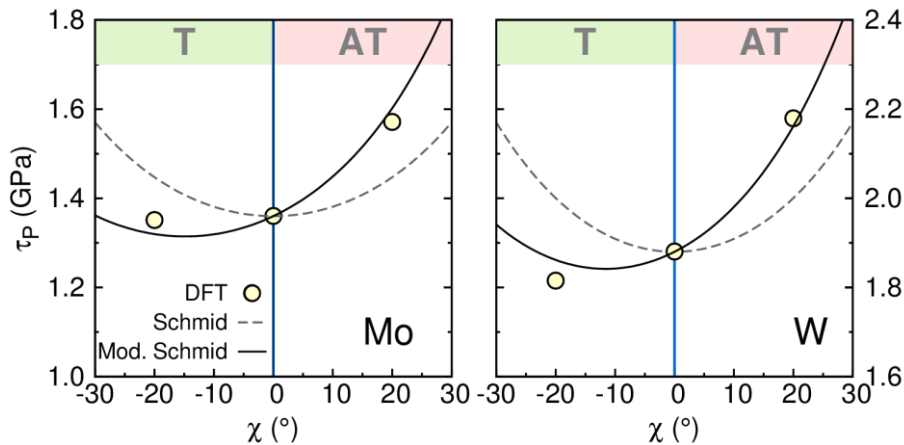

Supplementary Figure 2: Modified Schmid law applied to interatomic potentials. The predictions from the modified Schmid law (full line) is compared to the calculations from Ref. [2] (circles) and to the original Schmid law (dashed line). The interatomic potential is the Mendelev et al. Embedded Atom Method potential from Ref. [3].

Supplementary Figure 3: Reaction coordinates to evaluate Peierls barriers.
(a) Reference reaction coordinate, where both dislocations of the dipole move in the
same direction. (b) Illustration of the displacement in opposite directions for
dislocations under stress. (c) Reaction coordinate used in the present study, where
only one dislocation is moved. (d) Peierls energies in tungsten for the reference
(black) and present (red) reaction coordinates. In the latter case, the energy barrier is
shown before (dashed line) and after (solid line) elastic corrections. Note that for the
reference reaction coordinate, we show only the maximum of the Peierls energy,
which by symmetry is halfway along the path, because the definition of the
dislocation position requires that only one dislocation moves and can therefore not
be applied with the reference reaction coordinate. The reference Peierls energy was
shown to not require elastic correction in Ref. [1] since the elastic energy induced
when moving the two dislocations simultaneously does not exceed 1 meV/b.

**Supplementary Figure 4: Schmid law deviation obtained with the cost function
method.** The Peierls stress variations calculated with DFT under stress (circles) are
compared to the original Schmid law (dashed lines) and to the modified Schmid law
(full lines).

Supplementary Table 1: Deviation angle obtained from DFT calculations in absence of applied stress in all bcc transition metals evaluated with the cost function method.

	V	Nb	Ta	Mo	W	Fe
Cost function	-18.9	-24.7	-7.2	-14.9	-11.6	-5.3

Supplementary References

[1] Dezerald, L. *et al.* Ab initio modeling of the two-dimensional energy landscape of screw dislocations in bcc transition metals. *Phys. Rev. B* 89, 024104–13 (2014).

[2] Chaussidon, J., Fivel, M. & Rodney, D. The glide of screw dislocations in BCC Fe: Atomistic   static and dynamic simulations. *Acta Mater.* 54, 3407–3416 (2006).

[3] Mendelev, M. I. *et al.* Development of new interatomic potentials appropriate for crystalline and liquid iron. *Philos. Mag.* 83, 3977–3994 (2003).